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Crude oil characterization using TGA-DTA, TGA-FTIR and TGA-MS techniques

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ABSTRACT

In this research, combustion characterization and kinetics of four different origin crude oil samples were determined using thermogravimetry - differential thermal analysis (TGA-DTA) and thermogravimetry - Fourier transform infrared (TGA-FTIR) and thermogravimetry – mass spectrophotometry (TGA-MS) techniques.

In the TGA-DTA analysis of crude oil samples, low temperature oxidation (LTO) and high temperature oxidation (HTO) reaction regions were observed in different temperature intervals. On the other hand, reaction regions, mass loss, and peak-burnout temperatures of the crude oil samples were also determined using TGA-DTA curves. In TGA-FTIR analysis, spectrums of crude oil samples were examined at different time intervals and composition of several hydrocarbon compounds was determined quantitatively. This research was also focused on the main volatile products (H_2, H_2O, CO, CO, C_6H_6, SO_2 etc…) of different origin crude oil samples on the basis of both their relative intensities and on their relevancy by using TGA-MS technique.

Two different Arrhenius types of kinetic models were used in order to determine the kinetic triplets (activation energy, Arrhenius constant and reaction order) of crude oil samples studied. It was observed that in HTO region, higher activation energy values were observed depending on the °API gravities of the crude oils.

1. Introduction

Applications of thermal analysis techniques have advantages over other methods of investigation, being simpler to perform and more readily amenable to characterization and kinetic analysis from the point of in-situ combustion laboratory - studies and field applications. Much of the work on thermal analysis of crude oil was directed toward the oxidation and/or cracking-combustion behavior of the samples and kinetic studies by thermal research using differential scanning calorimeter (DSC), thermogravimetry -differential thermal analysis (TGA-DTA) and simultaneous thermogravimetry - Fourier transform infrared (TGA-FTIR). Applications of thermal analysis techniques have advantages over other methods of investigation, being simpler to perform and more readily amenable to characterization and kinetic analysis.

Thermogravimetry (TGA) and differential scanning calorimetry (DSC) was used by many authors to study the temperature intervals and corresponding reaction regions of different origin crude oils, such as distillation and others (Shiskin, 2006a, 2006b; Lukyaa et al., 1994; Li et al., 2006; Shiskin, 2006a, 2006b; Borchardt and Daniels, 1957; Trejo et al., 2010; Mahinpey et al., 2010a; Mahinpey et al., 2010b; Mehta et al., 2009; Goncalves et al., 2008). The pyrolysis and combustion properties of different origin and °API gravity of crude oils was characterized by thermogravimetry (TGA) and differential scanning calorimetry (DSC) in order to distinguish the reaction regions and corresponding kinetic data and the heat of reactions. Higher activation energy values were found as the °API gravity of the crude oil decreased (Kok, 2002; Kok, 2006; Kok, 2003; Kok et al., 2004). On the other hand, in another thermal study, properties of different origin crude oils were investigated by thermogravimetry- differential scanning calorimetry - Fourier transform infrared spectroscopy (TGA-DSC-FTIR) under nitrogen atmosphere to determine the inorganic components. It was observed that SO_3 concentration was highest in all the crude oils studied (Mothe et al., 2013a, 2013b, 2013c). Effect of different additives and salts was studied on the combustion properties of crude oils and it was concluded that depending on the composition and concentration of the metallic additives used, different effect on the kinetic parameters of the crude oils was observed (Li et al., 2013). In a comparative study on thermal characteristics of different crude oils was studied to determine the reaction regions, peak, and burnout temperatures. In the content of the study, the Arrhenius equation provided kinetic data, such as activation energy, pre-exponential factor, and order of the reaction (Mahinpey et al., 2010a, 2010b).

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